

Full wwPDB X-ray Structure Validation Report (i)

Jun 9, 2022 – 01:21 pm BST

PDB ID	:	7PPI
Title	:	Crystal STRUCTURE OF NAMPT IN COMPLEX WITH Compound 11
Authors	:	Hillig, R.C.
Deposited on	:	2021-09-13
Resolution	:	2.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.33 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Motria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	492	65%	27%	• 6%
1	В	492	5% 72%	21%	• 6%
1	С	492	3% 72%	20%	• 6%
1	D	492	4% 71%	21%	• 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	В	502	-	-	Х	-
3	PO4	D	502	-	-	Х	-
4	CL	А	505	-	-	Х	-
4	CL	В	503	-	-	Х	-
4	CL	С	505	-	-	Х	-

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16184 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	462	Total	С	Ν	0	S	0	0 0 0	0
	A	405	3703	2382	612	702	7	0	0	0
1	Р	462	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	D	405	3707	2386	612	702	7	0	1	U
1	C	464	Total	С	Ν	0	S	0	0	0
			3711	2388	613	703	7	0	0	0
1 D	462	Total	С	Ν	0	S	0	2	0	
	403	3712	2391	612	702	7	0		0	

• Molecule 1 is a protein called Nicotinamide phosphoribosyltransferase.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	GLY	-	expression tag	UNP P43490
В	0	GLY	-	expression tag	UNP P43490
С	0	GLY	-	expression tag	UNP P43490
D	0	GLY	-	expression tag	UNP P43490

• Molecule 2 is N-[4-[(5R)-1-(4-azanylbutyl)-6-oxidanylidene-5-quinolin-5-yl-4,5-dihydropyrid azin-3-yl]phenyl]-1,3-dihydropyrrolo[3,4-c]pyridine-2-carboxamide (three-letter code: 7Z2) (formula: C₃₁H₃₁N₇O₂) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	Λ	1	Total	С	Ν	0	0	0
	Л	T	40	31	7	2	0	0
2	В	1	Total	С	Ν	Ο	0	0
	2 В	1	40	31	7	2	0	0
0	С	1	Total	С	Ν	Ο	0	0
			40	31	7	2	0	0
2 D	1	Total	С	Ν	0	0	0	
	D	L	40	31	7	2	0	0

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	3	Total Cl 3 3	0	0
4	В	1	Total Cl 1 1	0	0
4	С	3	Total Cl 3 3	0	0

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	283	Total O 283 283	0	0
6	В	280	Total O 280 280	0	0
6	С	280	Total O 280 280	0	0
6	D	303	Total O 303 303	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Nicotinamide phosphoribosyltransferase



• Molecule 1: Nicotinamide phosphoribosyltransferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	82.21Å 106.26Å 120.95Å	Depositor
a, b, c, α , β , γ	90.00° 96.42° 90.00°	Depositor
Bosolution(A)	46.14 - 2.33	Depositor
	46.14 - 2.33	EDS
% Data completeness	95.3 (46.14-2.33)	Depositor
(in resolution range)	95.3(46.14-2.33)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	0.23	Depositor
$< I/\sigma(I) > 1$	$1.33 (at 2.32 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
B B.	0.292 , 0.359	Depositor
II, II, <i>free</i>	0.294 , 0.358	DCC
R_{free} test set	2100 reflections $(2.48%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	14.9	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$ < L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16184	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 68.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3190e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PO4, 7Z2, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal Chain		Bo	ond lengths	Bond angles	
	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.92	4/3791~(0.1%)	1.04	7/5138~(0.1%)
1	В	0.91	4/3798~(0.1%)	1.04	9/5148~(0.2%)
1	С	0.94	4/3799~(0.1%)	1.05	8/5149~(0.2%)
1	D	0.93	6/3806~(0.2%)	1.02	5/5159~(0.1%)
All	All	0.92	18/15194~(0.1%)	1.04	29/20594~(0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	258	GLU	CD-OE1	8.36	1.34	1.25
1	А	167	GLU	CD-OE2	7.71	1.34	1.25
1	D	246	GLU	CD-OE2	-7.24	1.17	1.25
1	В	258	GLU	CD-OE2	-7.17	1.17	1.25
1	С	445	GLU	CD-OE1	-6.95	1.18	1.25
1	D	178	GLU	CD-OE1	6.83	1.33	1.25
1	С	246	GLU	CD-OE2	-6.82	1.18	1.25
1	А	444	GLU	CD-OE1	6.58	1.32	1.25
1	В	336	GLU	CD-OE1	6.51	1.32	1.25
1	С	326	GLU	CD-OE2	6.15	1.32	1.25
1	С	398	SER	C-O	6.04	1.34	1.23
1	D	258	GLU	CD-OE2	5.88	1.32	1.25
1	D	258	GLU	CD-OE1	5.78	1.32	1.25
1	D	149	GLU	CD-OE2	5.76	1.31	1.25
1	В	56	GLU	CD-OE2	-5.65	1.19	1.25
1	A	288	GLU	CD-OE2	5.57	1.31	1.25
1	D	115	GLU	CD-OE2	-5.48	1.19	1.25
1	В	202	GLU	CD-OE1	-5.25	1.19	1.25

All (29) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	393	ASP	CB-CA-C	-8.27	93.86	110.40
1	С	40	ARG	NE-CZ-NH1	-7.97	116.31	120.30
1	D	349	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	В	40	ARG	NE-CZ-NH1	-7.15	116.72	120.30
1	С	184	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	В	434	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	А	195	TYR	CB-CG-CD1	6.41	124.85	121.00
1	С	40	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	В	18	TYR	CB-CG-CD1	6.00	124.60	121.00
1	А	18	TYR	CB-CG-CD1	5.75	124.45	121.00
1	В	40	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	В	434	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	D	18	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	В	184	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	В	196	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	В	393	ASP	CB-CA-C	-5.54	99.31	110.40
1	D	349	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	А	313	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	А	195	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	С	18	TYR	CB-CG-CD1	5.43	124.26	121.00
1	А	429	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	В	305	GLN	CB-CA-C	-5.36	99.68	110.40
1	С	349	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	А	483	ASN	CA-C-O	-5.26	109.06	120.10
1	С	127	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	396	ASN	CB-CA-C	5.18	120.77	110.40
1	D	18	TYR	CB-CG-CD1	5.14	124.08	121.00
1	D	9	PHE	CB-CA-C	-5.02	100.37	110.40
1	С	429	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3703	0	3675	106	0



7P	Pl

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	3707	0	3684	90	0
1	С	3711	0	3686	85	0
1	D	3712	0	3695	79	0
2	А	40	0	0	4	0
2	В	40	0	0	5	0
2	С	40	0	0	5	0
2	D	40	0	0	4	0
3	А	5	0	0	0	0
3	В	5	0	0	2	0
3	С	5	0	0	1	0
3	D	5	0	0	5	0
4	А	3	0	0	3	0
4	В	1	0	0	2	0
4	С	3	0	0	3	0
5	А	6	0	8	0	0
5	С	12	0	16	2	0
6	А	283	0	0	24	0
6	В	280	0	0	28	0
6	С	280	0	0	22	0
6	D	303	0	0	20	0
All	All	16184	0	14764	355	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (355) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (Å)
4:A:505:CL:CL	6:B:773:HOH:O	1.91	1.19
1:C:391:THR:CG2	1:C:393:ASP:HB2	1.89	1.03
1:D:398:SER:OG	3:D:502:PO4:O4	1.78	1.00
1:A:391:THR:HG23	1:A:393:ASP:H	1.26	0.98
1:C:32:LYS:NZ	1:C:135:GLU:OE2	2.01	0.94
1:C:391:THR:HG22	1:C:393:ASP:HB2	1.48	0.94
1:A:272:VAL:HG22	1:A:273:PRO:HD2	1.50	0.92
1:B:216:LYS:HE3	6:B:744:HOH:O	1.71	0.91
1:D:114:ILE:HD11	1:D:144:LEU:HG	1.51	0.91
1:D:104:ILE:HD11	1:D:141:CYS:SG	2.11	0.89
4:C:505:CL:CL	6:D:774:HOH:O	2.27	0.89
4:A:505:CL:CL	6:A:668:HOH:O	2.35	0.81
1:D:264:HIS:O	1:D:268:GLN:HG2	1.80	0.80



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:A:505:CL:CL	1:B:311:ARG:NH2	2.51	0.79
1:B:459:HIS:HB3	6:B:809:HOH:O	1.81	0.79
4:B:503:CL:CL	6:B:802:HOH:O	2.36	0.79
1:A:441:VAL:HG11	1:A:453:TYR:CE2	2.19	0.78
4:C:506:CL:CL	6:C:813:HOH:O	2.39	0.77
1:A:56:GLU:OE1	1:A:166:ARG:NH1	2.17	0.77
1:A:391:THR:CG2	1:A:393:ASP:H	1.96	0.77
1:B:357:ASP:OD2	6:B:601:HOH:O	2.01	0.77
3:B:502:PO4:O2	6:B:602:HOH:O	2.01	0.76
1:D:374:SER:OG	1:D:376:GLU:HG2	1.85	0.76
1:C:174:LYS:HE2	1:C:175:TYR:CE2	2.20	0.75
4:C:505:CL:CL	6:D:863:HOH:O	2.41	0.75
1:A:149:GLU:OE2	6:A:601:HOH:O	2.05	0.75
1:A:38:GLU:OE2	1:A:40:ARG:HA	1.88	0.73
1:B:391:THR:OG1	1:B:393:ASP:HB2	1.89	0.72
1:B:434:ARG:HD2	1:B:457:LEU:HD21	1.71	0.72
1:C:391:THR:HG23	1:C:393:ASP:H	1.54	0.71
1:D:104:ILE:CD1	1:D:141:CYS:SG	2.78	0.71
1:B:334[A]:VAL:HG22	6:B:665:HOH:O	1.88	0.71
1:B:211:HIS:HB2	1:B:386:LEU:HD21	1.72	0.70
1:A:175:TYR:HB3	1:A:375:ILE:HG13	1.72	0.70
1:A:430:LEU:O	6:A:602:HOH:O	2.08	0.70
1:B:217:GLY:HA3	6:B:722:HOH:O	1.93	0.69
1:C:357:ASP:OD2	1:C:389:LYS:NZ	2.27	0.68
1:B:216:LYS:CE	6:B:744:HOH:O	2.36	0.67
1:D:175:TYR:HB3	1:D:375:ILE:HG13	1.78	0.67
1:B:41:GLU:OE2	1:B:422:ASN:ND2	2.28	0.66
1:C:392:ARG:HD3	1:D:197:GLY:HA2	1.77	0.66
1:B:175:TYR:HB3	1:B:375:ILE:HG13	1.78	0.66
1:C:391:THR:CG2	1:C:393:ASP:H	2.08	0.66
1:C:391:THR:HG21	1:C:393:ASP:HB2	1.76	0.66
1:A:466:LYS:HE2	6:A:855:HOH:O	1.96	0.66
1:A:469:LYS:HE3	1:A:471:TYR:CZ	2.31	0.66
2:B:501:7Z2:C35	2:B:501:7Z2:O31	2.45	0.64
1:C:175:TYR:HB3	1:C:375:ILE:HG13	1.80	0.64
1:C:37:PHE:CZ	1:C:397:CYS:HB3	2.33	0.63
1:A:444:GLU:OE2	6:A:603:HOH:O	2.15	0.63
1:C:96:PHE:O	5:C:507:GOL:H32	1.98	0.63
1:A:66:LEU:HD23	1:A:70:LEU:HD12	1.80	0.62
1:D:333:PRO:HA	6:D:718:HOH:O	1.98	0.62
1:D:400:LYS:NZ	3:D:502:PO4:O4	2.32	0.62



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:40:ARG:NE	1:A:422:ASN:O	2.29	0.62
1:A:374:SER:OG	1:A:376:GLU:HG2	1.99	0.62
1:C:304:THR:HB	6:C:847:HOH:O	2.00	0.61
1:B:211:HIS:CG	1:B:386:LEU:HD21	2.35	0.61
1:B:434:ARG:HG3	1:B:434:ARG:HH21	1.65	0.61
1:C:202:GLU:HA	6:C:720:HOH:O	2.00	0.61
1:D:458:LEU:HD12	6:D:707:HOH:O	1.99	0.61
1:C:398:SER:OG	3:C:502:PO4:O2	2.10	0.61
1:D:242:VAL:HG22	2:D:501:7Z2:C40	2.31	0.61
1:A:412:ASN:HB2	6:A:743:HOH:O	2.01	0.61
1:A:92:GLN:HA	1:A:92:GLN:NE2	2.16	0.60
1:A:173:ALA:HA	1:A:183:LEU:CD2	2.31	0.60
1:A:31:SER:O	1:A:139:PRO:HA	2.01	0.59
1:C:455:GLN:NE2	6:C:613:HOH:O	2.34	0.59
1:A:258:GLU:OE2	6:A:604:HOH:O	2.16	0.59
1:A:441:VAL:CG1	1:A:453:TYR:CE2	2.85	0.59
1:C:376:GLU:HA	6:C:697:HOH:O	2.01	0.59
1:A:24:LYS:HB3	1:B:268:GLN:HG2	1.85	0.59
1:D:41:GLU:OE2	1:D:422:ASN:ND2	2.35	0.59
1:A:174:LYS:O	1:A:178:GLU:HG3	2.03	0.58
3:B:502:PO4:O1	6:B:603:HOH:O	2.15	0.58
1:B:343:LEU:CD1	1:B:376:GLU:HG3	2.33	0.58
1:C:391:THR:CG2	1:C:393:ASP:CB	2.74	0.58
1:D:398:SER:HG	1:D:400:LYS:HZ3	1.47	0.58
1:B:17:SER:OG	1:B:90:HIS:NE2	2.34	0.58
1:B:31:SER:O	1:B:139:PRO:HA	2.03	0.58
1:C:31:SER:O	1:C:139:PRO:HA	2.03	0.58
1:B:184:ASP:HB2	6:B:764:HOH:O	2.04	0.57
1:A:130:VAL:HG12	1:A:442:THR:HG23	1.87	0.57
1:C:258:GLU:OE2	6:C:601:HOH:O	2.17	0.57
1:C:189:LYS:HE3	1:C:375:ILE:HG22	1.86	0.57
1:C:374:SER:OG	1:C:376:GLU:HG2	2.05	0.57
1:A:398:SER:OG	1:A:400:LYS:NZ	2.33	0.57
1:A:258:GLU:HB3	6:A:604:HOH:O	2.06	0.56
1:D:31:SER:O	1:D:139:PRO:HA	2.04	0.56
1:D:412:ASN:OD1	6:D:601:HOH:O	2.17	0.56
1:D:189:LYS:NZ	2:D:501:7Z2:N26	2.53	0.56
1:A:57:THR:HG21	1:A:395:LEU:HD13	1.86	0.56
1:B:433:HIS:HB3	1:B:453:TYR:HB3	1.87	0.56
1:B:418:VAL:N	6:B:613:HOH:O	2.40	0.55
1:B:62:LEU:HD12	1:B:62:LEU:O	2.07	0.55



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:70:LEU:HD11	1:B:152:LEU:HD21	1.87	0.55
4:B:503:CL:CL	6:B:706:HOH:O	2.56	0.55
1:B:374:SER:OG	1:B:376:GLU:HG2	2.06	0.54
1:A:391:THR:CG2	1:A:393:ASP:N	2.68	0.54
1:D:69:TYR:OH	1:D:202:GLU:OE2	2.25	0.54
1:B:279:ASP:OD2	6:B:604:HOH:O	2.18	0.54
1:A:11:ILE:HG22	6:A:609:HOH:O	2.07	0.54
1:D:189:LYS:HE3	1:D:375:ILE:HG22	1.89	0.54
1:A:16:ASP:OD2	1:B:196:ARG:NH2	2.39	0.54
1:D:469:LYS:NZ	1:D:471:TYR:OH	2.23	0.54
1:A:349:ARG:CZ	6:A:661:HOH:O	2.56	0.53
1:B:211:HIS:CB	1:B:386:LEU:HD21	2.37	0.53
1:B:379:ALA:HB2	2:B:501:7Z2:C25	2.37	0.53
1:C:219:ASP:HA	1:D:17:SER:OG	2.08	0.53
1:C:343:LEU:CD1	1:C:376:GLU:HG3	2.39	0.53
1:B:130:VAL:HG12	1:B:442:THR:HG23	1.91	0.52
1:A:272:VAL:HG22	1:A:273:PRO:CD	2.31	0.52
2:D:501:7Z2:C29	2:D:501:7Z2:C30	2.87	0.52
1:C:174:LYS:HE2	1:C:175:TYR:CZ	2.44	0.52
1:A:24:LYS:HD3	1:B:268:GLN:OE1	2.10	0.52
1:C:211:HIS:CG	1:C:386:LEU:HD11	2.45	0.52
1:A:447:LYS:HE3	6:A:869:HOH:O	2.10	0.52
1:B:189:LYS:HE3	1:B:375:ILE:HG22	1.91	0.52
1:B:211:HIS:ND1	1:B:386:LEU:HD21	2.25	0.51
1:B:244:ALA:CB	1:B:275:SER:HB3	2.40	0.51
1:A:54:TYR:OH	1:A:164:ASN:OD1	2.27	0.51
1:A:338:SER:HB3	6:A:676:HOH:O	2.11	0.51
1:B:211:HIS:HB2	1:B:386:LEU:CD2	2.41	0.51
1:D:382:SER:HB3	1:D:386:LEU:HB2	1.92	0.51
2:C:501:7Z2:C29	2:C:501:7Z2:C30	2.89	0.51
1:C:251:THR:O	6:C:603:HOH:O	2.19	0.51
1:C:366:GLU:OE1	6:C:602:HOH:O	2.19	0.51
1:B:311:ARG:NH1	6:B:632:HOH:O	2.40	0.51
1:C:391:THR:HG22	1:C:393:ASP:CB	2.31	0.51
1:A:244:ALA:HA	1:A:275:SER:O	2.10	0.50
2:A:501:7Z2:C29	2:A:501:7Z2:C30	2.89	0.50
1:A:323:LYS:HD3	6:A:711:HOH:O	2.11	0.50
1:A:290:ILE:HD11	6:A:604:HOH:O	2.12	0.50
1:C:236:PRO:HD2	6:C:773:HOH:O	2.11	0.50
1:C:288:GLU:O	1:C:293:GLU:HG3	2.12	0.50
1:A:256:ASP:C	6:A:654:HOH:O	2.50	0.50



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:402:SER:O	1:B:428:GLY:N	2.42	0.50
1:B:429:ARG:HD3	6:B:817:HOH:O	2.12	0.50
1:A:402:SER:O	1:A:428:GLY:N	2.44	0.50
1:A:10:ASN:HB3	1:A:13:LEU:HD12	1.93	0.50
1:D:460:THR:HG21	6:D:879:HOH:O	2.11	0.50
1:B:351:ILE:HD12	1:B:379:ALA:HB3	1.94	0.49
1:B:420:ASP:OD1	1:B:422:ASN:HB2	2.12	0.49
1:D:427:LYS:HG3	6:D:639:HOH:O	2.12	0.49
1:C:130:VAL:HG12	1:C:442:THR:HG23	1.94	0.49
1:B:379:ALA:HB2	2:B:501:7Z2:C24	2.42	0.49
2:B:501:7Z2:C30	2:B:501:7Z2:C29	2.90	0.49
1:B:351:ILE:HD12	1:B:379:ALA:CB	2.42	0.49
1:C:196:ARG:NH2	1:D:16:ASP:OD2	2.46	0.49
1:D:399:PHE:O	6:D:602:HOH:O	2.19	0.49
1:A:92:GLN:HA	1:A:92:GLN:HE21	1.74	0.49
1:C:423:LYS:NZ	1:D:354:ASP:OD1	2.44	0.49
1:A:183:LEU:HD22	1:A:186:LEU:HD22	1.95	0.49
1:B:389:LYS:HE2	6:B:831:HOH:O	2.12	0.49
1:C:399:PHE:O	1:C:400:LYS:HD3	2.13	0.49
1:A:424:ARG:HH11	1:A:424:ARG:HG2	1.77	0.49
1:C:176:LEU:HD11	6:C:697:HOH:O	2.12	0.49
1:A:192:ASP:CG	1:A:220:THR:HG1	2.17	0.48
1:C:70:LEU:HD11	1:C:152:LEU:HD21	1.94	0.48
1:A:189:LYS:HE3	1:A:375:ILE:HG22	1.94	0.48
1:D:178:GLU:HG2	1:D:369:LYS:HE3	1.96	0.48
1:A:379:ALA:HB2	2:A:501:7Z2:C25	2.44	0.48
1:D:233:THR:HG22	1:D:473:PHE:HB3	1.96	0.48
1:A:194:GLY:CA	1:A:383:GLY:HA2	2.43	0.48
1:C:197:GLY:HA2	1:D:392:ARG:HD3	1.95	0.48
1:D:81:GLN:NE2	1:D:85:ASP:OD1	2.47	0.48
1:A:453:TYR:C	1:A:454:GLY:O	2.52	0.48
1:A:27:PRO:HA	1:B:253:TRP:CZ2	2.49	0.48
1:A:244:ALA:CB	1:A:275:SER:HB3	2.44	0.48
1:A:392:ARG:NE	1:B:196:ARG:HG3	2.29	0.48
1:B:68:LYS:HA	6:B:778:HOH:O	2.14	0.48
1:C:309:ILE:HG22	1:C:351:ILE:HG22	1.95	0.48
1:C:244:ALA:CB	1:C:275:SER:HB3	2.44	0.47
1:D:217:GLY:HA3	6:D:691:HOH:O	2.13	0.47
1:D:242:VAL:HG22	2:D:501:7Z2:C39	2.44	0.47
1:D:368:MET:SD	1:D:378:ILE:HG21	2.54	0.47
1:A:382:SER:HB3	1:A:386:LEU:HB2	1.95	0.47



Atom-1 Atom-2		Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:D:114:ILE:HD12	1:D:148:ILE:HD11	1.95	0.47
1:A:132:PHE:HE2	1:A:152:LEU:HD13	1.80	0.47
1:A:481:GLN:NE2	6:A:643:HOH:O	2.47	0.47
1:B:134:VAL:HG21	1:B:152:LEU:CD1	2.45	0.47
1:B:343:LEU:HD11	1:B:376:GLU:HG3	1.95	0.47
1:A:309:ILE:HG22	1:A:351:ILE:HG22	1.96	0.47
1:D:402:SER:O	1:D:428:GLY:N	2.43	0.47
1:A:193:PHE:CE2	1:A:381:GLY:HA3	2.50	0.47
1:D:99:LYS:HD2	6:D:743:HOH:O	2.14	0.47
1:A:198:VAL:CG1	1:A:387:LEU:HB3	2.45	0.47
1:D:130:VAL:HG12	1:D:442:THR:HG23	1.97	0.47
1:A:40:ARG:NE	1:A:423:LYS:HA	2.30	0.47
1:A:113:PRO:HD2	1:A:144:LEU:CD2	2.44	0.47
1:C:246:GLU:OE2	1:D:22:HIS:CE1	2.68	0.47
1:A:326:GLU:HG3	6:A:800:HOH:O	2.15	0.46
1:B:37:PHE:CZ	1:B:397:CYS:HB3	2.50	0.46
1:B:169:LYS:HG2	1:B:482:LEU:HD11	1.98	0.46
1:C:216:LYS:O	1:C:239:GLY:HA2	2.15	0.46
1:A:173:ALA:HA	1:A:183:LEU:HD21	1.96	0.46
1:B:392:ARG:NH1	6:B:644:HOH:O	2.49	0.46
1:D:194:GLY:CA	1:D:383:GLY:HA2	2.46	0.46
1:D:244:ALA:HA	1:D:275:SER:O	2.15	0.46
1:D:189:LYS:HZ1	1:D:376:GLU:HA	1.81	0.46
1:D:333:PRO:O	1:D:345:PRO:HD3	2.16	0.46
1:D:400:LYS:HZ1	3:D:502:PO4:P	2.38	0.46
1:A:21:THR:HG21	1:B:243:PRO:HA	1.98	0.46
1:C:484:ILE:O	1:C:484:ILE:HG13	2.16	0.46
1:C:99:LYS:HD2	5:C:507:GOL:O1	2.15	0.46
1:A:40:ARG:HD3	6:A:832:HOH:O	2.15	0.45
1:A:244:ALA:HB2	1:A:275:SER:HB3	1.98	0.45
1:A:441:VAL:HG11	1:A:453:TYR:CZ	2.49	0.45
1:A:63:GLN:NE2	1:A:230:TYR:O	2.50	0.45
1:A:219:ASP:HA	1:B:17:SER:HB2	1.98	0.45
1:B:123:PHE:HB3	1:B:125:ILE:HD11	1.97	0.45
1:B:474:ASP:OD1	6:B:605:HOH:O	2.21	0.45
1:C:391:THR:HG23	6:C:843:HOH:O	2.15	0.45
1:B:456:ASP:HB2	6:B:823:HOH:O	2.16	0.45
1:C:242:VAL:HG22	2:C:501:7Z2:C40	2.46	0.45
1:C:409:LEU:HD12	6:C:766:HOH:O	2.15	0.45
1:A:199:SER:O	1:A:200:SER:HB3	2.16	0.45
1:A:255:LYS:HA	1:A:281:TYR:CZ	2.52	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:391:THR:CG2	1:A:393:ASP:HB2	2.47	0.45
1:B:309:ILE:HG22	1:B:351:ILE:HG22	1.99	0.45
1:C:19:LYS:HA	1:C:22:HIS:ND1	2.31	0.45
1:D:216:LYS:O	1:D:239:GLY:HA2	2.16	0.45
1:C:293:GLU:OE2	1:C:331:LYS:NZ	2.29	0.45
1:A:259:LYS:HD2	1:A:294:ASP:HB3	1.99	0.45
1:B:194:GLY:CA	1:B:383:GLY:HA2	2.46	0.45
1:B:193:PHE:CZ	2:B:501:7Z2:C6	2.99	0.45
1:B:418:VAL:HG12	6:B:613:HOH:O	2.16	0.45
1:C:349:ARG:HB3	2:C:501:7Z2:C24	2.47	0.45
1:D:66:LEU:HD23	1:D:70:LEU:HD12	1.98	0.45
1:C:389:LYS:HE2	6:C:826:HOH:O	2.15	0.45
1:D:103:TYR:O	1:D:107:LYS:HB2	2.15	0.45
1:C:117:LYS:HA	1:C:459:HIS:O	2.17	0.45
1:C:402:SER:O	1:C:428:GLY:N	2.44	0.45
1:A:117:LYS:HA	1:A:459:HIS:O	2.17	0.44
1:A:413:VAL:HG11	1:B:252:ALA:HA	1.99	0.44
2:A:501:7Z2:O11	2:A:501:7Z2:C14	2.64	0.44
1:B:464:ASN:HA	6:B:688:HOH:O	2.17	0.44
1:C:194:GLY:CA	1:C:383:GLY:HA2	2.47	0.44
1:C:415:LYS:NZ	6:C:606:HOH:O	2.26	0.44
1:A:92:GLN:NE2	1:A:92:GLN:CA	2.81	0.44
1:A:13:LEU:HD11	1:A:82:GLU:OE2	2.18	0.44
1:B:19:LYS:HA	1:B:22:HIS:ND1	2.33	0.44
1:D:193:PHE:CE2	1:D:381:GLY:HA3	2.52	0.44
1:B:81:GLN:HE22	1:B:84:LYS:HD3	1.82	0.44
1:B:278:SER:O	1:B:283:ILE:HA	2.18	0.44
1:B:466:LYS:HA	6:B:794:HOH:O	2.16	0.44
1:C:329:GLY:HA2	1:C:334:VAL:CG2	2.47	0.44
1:B:9:PHE:N	6:B:645:HOH:O	2.49	0.44
1:C:23:TYR:CE1	1:C:97:ASN:HB2	2.53	0.44
1:C:443:LEU:HA	6:C:629:HOH:O	2.16	0.44
1:A:199:SER:HB2	1:B:157:TYR:CD2	2.53	0.44
1:C:388:GLN:NE2	1:D:156:TRP:HH2	2.16	0.44
1:D:398:SER:CB	3:D:502:PO4:O4	2.64	0.44
1:A:19:LYS:HA	1:A:22:HIS:ND1	2.32	0.44
1:A:66:LEU:HD13	1:A:462:PHE:HB2	2.00	0.44
1:C:333:PRO:O	1:C:345:PRO:HD3	2.17	0.44
1:D:103:TYR:CE1	1:D:107:LYS:HG3	2.53	0.44
1:D:469:LYS:HE2	6:D:714:HOH:O	2.16	0.44
1:A:116:ILE:HA	1:A:133:THR:O	2.17	0.43



Atom 1 Atom 2		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:277:VAL:HA	1:A:311:ARG:HB3	2.00	0.43	
1:A:57:THR:CG2	1:A:395:LEU:HD13	2.48	0.43	
1:C:74:VAL:HG12	6:C:621:HOH:O	2.18	0.43	
1:C:198:VAL:CG1	1:C:387:LEU:HB3	2.48	0.43	
1:C:278:SER:O	1:C:283:ILE:HA	2.18	0.43	
1:C:344:LEU:HD22	1:C:348:LEU:HD23	2.00	0.43	
1:D:120:PRO:HB2	1:D:123:PHE:CD1	2.53	0.43	
1:D:198:VAL:CG1	1:D:387:LEU:HB3	2.48	0.43	
1:C:18:TYR:HB3	6:D:723:HOH:O	2.17	0.43	
1:C:418:VAL:HG12	6:C:723:HOH:O	2.18	0.43	
1:B:37:PHE:HZ	1:B:397:CYS:HB3	1.83	0.43	
1:B:117:LYS:HA	1:B:459:HIS:O	2.19	0.43	
1:D:23:TYR:CE1	1:D:97:ASN:HB2	2.53	0.43	
1:D:120:PRO:O	1:D:123:PHE:HB2	2.17	0.43	
1:A:391:THR:HG23	1:A:393:ASP:N	2.10	0.43	
1:B:114:ILE:HD13	1:B:136:ASN:HA	2.01	0.43	
1:D:230:TYR:HE2	6:D:888:HOH:O	2.02	0.43	
1:B:433:HIS:CD2	1:B:443:LEU:HD12	2.53	0.43	
1:C:283:ILE:HG23	1:C:284:TYR:N	2.34	0.43	
1:C:472:SER:HB2	6:C:686:HOH:O	2.18	0.43	
1:D:177[A]:LEU:HD22	1:D:177[A]:LEU:HA	1.91	0.43	
1:B:243:PRO:O	1:B:274:VAL:HA	2.19	0.43	
1:B:277:VAL:HA	1:B:311:ARG:HB3	2.01	0.43	
1:C:382:SER:HB3	1:C:386:LEU:HB2	2.01	0.43	
1:B:209:SER:HA	1:B:227:ILE:HD11	2.00	0.43	
1:B:345:PRO:HG2	1:B:347:TYR:CE1	2.54	0.43	
1:B:434:ARG:NE	6:B:628:HOH:O	2.38	0.43	
1:D:410:GLY:HA3	6:D:818:HOH:O	2.19	0.43	
1:A:209:SER:HA	1:A:227:ILE:HD11	2.00	0.42	
1:B:116:ILE:HA	1:B:133:THR:O	2.19	0.42	
1:D:323:LYS:NZ	6:D:627:HOH:O	2.42	0.42	
1:D:333:PRO:HD2	1:D:345:PRO:HG3	2.01	0.42	
2:A:501:7Z2:C27	6:A:813:HOH:O	2.67	0.42	
1:A:199:SER:HB3	1:B:157:TYR:CD1	2.54	0.42	
1:C:174:LYS:HG3	6:C:879:HOH:O	2.18	0.42	
1:C:345:PRO:HG2	1:C:347:TYR:CE1	2.54	0.42	
1:C:423:LYS:NZ	6:C:610:HOH:O	2.30	0.42	
1:A:17:SER:O	1:A:20:VAL:HB	2.19	0.42	
1:B:333:PRO:HD2	1:B:345:PRO:HG3	2.02	0.42	
1:B:140:GLU:OE1	1:B:140:GLU:HA	2.20	0.42	
1:B:474:ASP:O	1:B:478:LYS:HD2	2.19	0.42	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:244:ALA:HA	1:C:275:SER:O	2.20	0.42	
1:D:116:ILE:HA	1:D:133:THR:O	2.19	0.42	
1:D:300:VAL:HG12	1:D:347:TYR:OH	2.20	0.42	
1:A:192:ASP:OD2	1:A:220:THR:HB	2.19	0.42	
1:A:338:SER:CB	6:A:676:HOH:O	2.68	0.42	
1:D:19:LYS:HA	1:D:22:HIS:ND1	2.35	0.42	
1:A:329:GLY:HA2	1:A:334:VAL:CG2	2.50	0.42	
1:A:176:LEU:HD13	1:A:189:LYS:HE3	2.00	0.42	
1:D:424:ARG:NH1	6:D:639:HOH:O	2.53	0.42	
1:C:242:VAL:HG22	2:C:501:7Z2:C39	2.50	0.42	
1:A:120:PRO:O	1:A:123:PHE:HB2	2.20	0.41	
1:D:32:LYS:HE2	1:D:32:LYS:HB2	1.82	0.41	
1:C:201:GLN:NE2	1:D:154:GLN:OE1	2.48	0.41	
1:A:224:LEU:HB2	6:A:657:HOH:O	2.19	0.41	
1:A:321:VAL:HG23	1:A:352:GLN:HE21	1.85	0.41	
1:A:333:PRO:O	1:A:345:PRO:HD3	2.21	0.41	
1:B:172:LEU:HD13	1:B:189:LYS:HB3	2.01	0.41	
1:C:443:LEU:HD11	1:C:453:TYR:CD2	2.55	0.41	
1:D:426:LYS:HA	6:D:639:HOH:O	2.19	0.41	
1:A:38:GLU:OE2	1:A:128:GLY:HA2	2.20	0.41	
1:D:282:ASP:N	6:D:614:HOH:O	2.34	0.41	
1:C:259:LYS:CE	1:C:294:ASP:HB3	2.50	0.41	
1:D:109:ASP:CG	6:D:690:HOH:O	2.58	0.41	
1:D:283:ILE:HG23	1:D:284:TYR:N	2.36	0.41	
1:A:253:TRP:CZ2	1:B:27:PRO:HA	2.56	0.41	
1:A:386:LEU:HD13	1:A:387:LEU:HD23	2.03	0.41	
1:B:329:GLY:HA2	1:B:334[A]:VAL:CG1	2.50	0.41	
1:B:244:ALA:HA	1:B:275:SER:O	2.21	0.41	
1:C:465:GLY:HA2	6:C:694:HOH:O	2.20	0.41	
1:A:268:GLN:NE2	1:A:268:GLN:HA	2.35	0.41	
1:A:277:VAL:N	6:A:611:HOH:O	2.32	0.41	
1:A:438:GLY:HA3	6:A:845:HOH:O	2.21	0.41	
1:B:422:ASN:HB3	6:B:757:HOH:O	2.20	0.41	
1:D:117:LYS:HA	1:D:459:HIS:O	2.21	0.41	
1:A:216:LYS:O	1:A:239:GLY:HA2	2.20	0.41	
1:C:202:GLU:HB2	6:D:804:HOH:O	2.21	0.41	
1:D:309:ILE:HG22	1:D:351:ILE:HG22	2.03	0.41	
1:A:37:PHE:CG	1:A:132:PHE:CE1	3.09	0.40	
1:A:257:HIS:N	6:A:654:HOH:O	2.53	0.40	
1:B:425:SER:HB2	6:B:637:HOH:O	2.20	0.40	
1:C:430:LEU:HD23	1:C:444:GLU:HA	2.03	0.40	



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
2:C:501:7Z2:C10	1:D:18:TYR:CE1	3.04	0.40
1:D:168:GLN:HG3	1:D:358:ILE:HD12	2.03	0.40
1:D:400:LYS:NZ	3:D:502:PO4:P	2.94	0.40
1:C:391:THR:CG2	1:C:393:ASP:N	2.80	0.40
1:C:413:VAL:HG11	1:D:252:ALA:HA	2.03	0.40
1:A:92:GLN:HE21	1:A:92:GLN:CA	2.35	0.40
1:C:418:VAL:HG21	1:D:282:ASP:OD2	2.21	0.40
1:D:67:ASN:HA	1:D:71:LYS:HD3	2.03	0.40
1:B:23:TYR:CE1	1:B:97:ASN:HB2	2.56	0.40
1:B:329:GLY:HA2	1:B:334[B]:VAL:CG2	2.52	0.40
1:C:332:PHE:CD2	1:C:348:LEU:CD2	3.05	0.40
1:A:332:PHE:CD2	1:A:348:LEU:CD2	3.05	0.40
1:B:333:PRO:O	1:B:345:PRO:HD3	2.21	0.40
1:C:424:ARG:NH2	6:C:653:HOH:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	459/492~(93%)	435~(95%)	23~(5%)	1 (0%)	47	55
1	В	460/492~(94%)	443 (96%)	17 (4%)	0	100	100
1	С	460/492~(94%)	437 (95%)	23~(5%)	0	100	100
1	D	461/492~(94%)	442 (96%)	18 (4%)	1 (0%)	47	55
All	All	1840/1968~(94%)	1757 (96%)	81 (4%)	2 (0%)	51	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
1	А	454	GLY	



Continued from previous page...

Mol	Chain	Res	Type
1	D	481	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	407/430~(95%)	391~(96%)	16 (4%)	32 41
1	В	408/430~(95%)	393~(96%)	15 (4%)	34 43
1	С	408/430~(95%)	391~(96%)	17 (4%)	30 37
1	D	409/430~(95%)	395~(97%)	14 (3%)	37 46
All	All	1632/1720~(95%)	1570 (96%)	62 (4%)	34 41

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	18	TYR
1	А	32	LYS
1	А	57	THR
1	А	77	LYS
1	А	190	LEU
1	А	195	TYR
1	А	196	ARG
1	А	234	LYS
1	А	235	ASP
1	А	248	SER
1	А	255	LYS
1	А	279	ASP
1	А	391	THR
1	А	393	ASP
1	А	455	GLN
1	А	469	LYS
1	В	18	TYR
1	В	32	LYS
1	В	41	GLU
1	В	155	SER



Mol	Chain	Res	Type
1	В	183	LEU
1	В	190	LEU
1	В	195	TYR
1	В	248	SER
1	В	255	LYS
1	В	299	ILE
1	В	333	PRO
1	В	338	SER
1	В	386	LEU
1	В	434	ARG
1	В	457	LEU
1	С	18	TYR
1	С	24	LYS
1	С	32	LYS
1	С	102	ASN
1	С	174	LYS
1	С	190	LEU
1	С	195	TYR
1	С	235	ASP
1	С	248	SER
1	С	303	SER
1	С	304	THR
1	С	391	THR
1	С	398	SER
1	С	400	LYS
1	С	451	GLU
1	С	455	GLN
1	С	470	SER
1	D	18	TYR
1	D	32	LYS
1	D	41	GLU
1	D	77	LYS
1	D	177[A]	LEU
1	D	177[B]	LEU
1	D	195	TYR
1	D	196	ARG
1	D	219	ASP
1	D	248	SER
1	D	275	SER
1	D	393	ASP
1	D	427	LYS
1	D	434	ARG

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	92	GLN
1	А	268	GLN
1	А	481	GLN
1	В	81	GLN
1	В	481	GLN
1	С	268	GLN
1	С	305	GLN
1	D	285	ASN
1	D	396	ASN
1	D	422	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Turne	Chain	Dec	T in le	Bond lengths			Bond angles			
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
2	7Z2	А	501	-	43,45,45	1.77	7 (16%)	49,63,63	1.88	14 (28%)	
5	GOL	С	504	-	$5,\!5,\!5$	0.16	0	$5,\!5,\!5$	0.42	0	



Mal	Turne	Chain	Dec	Tink	B	Bond lengths			Bond angles			
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
5	GOL	С	507	-	$5,\!5,\!5$	0.13	0	$5,\!5,\!5$	0.30	0		
3	PO4	D	502	-	4,4,4	0.74	0	6,6,6	0.61	0		
2	7Z2	D	501	-	43,45,45	1.76	9 (20%)	49,63,63	1.89	13 (26%)		
3	PO4	В	502	-	4,4,4	1.00	0	6,6,6	0.57	0		
5	GOL	А	504	-	$5,\!5,\!5$	0.11	0	$5,\!5,\!5$	0.16	0		
3	PO4	С	502	-	4,4,4	0.62	0	6,6,6	0.64	0		
3	PO4	А	502	-	4,4,4	0.82	0	6,6,6	0.63	0		
2	7Z2	С	501	-	43,45,45	1.81	11 (25%)	49,63,63	2.60	15 (30%)		
2	7Z2	В	501	-	43,45,45	1.93	8 (18%)	49,63,63	2.79	17 (34%)		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	С	504	-	-	4/4/4/4	-
5	GOL	С	507	-	-	2/4/4/4	-
2	7Z2	D	501	-	-	5/21/45/45	0/6/6/6
5	GOL	А	504	-	-	0/4/4/4	-
2	7Z2	С	501	-	-	5/21/45/45	0/6/6/6
2	7Z2	А	501	-	-	4/21/45/45	0/6/6/6
2	7Z2	В	501	-	-	8/21/45/45	0/6/6/6

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	501	7Z2	C16-C17	-5.93	1.36	1.47
2	А	501	7Z2	C17-N33	5.17	1.38	1.29
2	D	501	7Z2	N32-N33	-5.00	1.25	1.37
2	В	501	7Z2	N32-N33	-4.92	1.25	1.37
2	А	501	7Z2	N32-N33	-4.81	1.25	1.37
2	А	501	7Z2	C6-C5	4.71	1.56	1.50
2	С	501	7Z2	N32-N33	-4.54	1.26	1.37
2	\mathbf{C}	501	7Z2	C17-N33	4.33	1.36	1.29
2	С	501	7Z2	C16-C17	-4.27	1.39	1.47
2	D	501	7Z2	C17-N33	4.19	1.36	1.29
2	В	501	7Z2	C34-N32	3.96	1.52	1.46
2	A	501	7Z2	C13-N12	-3.78	1.34	1.41
2	D	501	7Z2	C6-C5	3.63	1.55	1.50

All (35) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	D	501	7Z2	C16-C17	-3.61	1.40	1.47
2	D	501	7Z2	C13-N12	-3.11	1.35	1.41
2	D	501	7Z2	C1-N2	-3.10	1.30	1.36
2	D	501	7Z2	C3-C4	3.10	1.54	1.50
2	В	501	7Z2	C13-N12	-3.05	1.35	1.41
2	В	501	7Z2	C17-N33	2.98	1.34	1.29
2	В	501	7Z2	C23-C22	-2.93	1.36	1.41
2	А	501	7Z2	C16-C17	-2.80	1.42	1.47
2	С	501	7Z2	C6-C5	2.79	1.54	1.50
2	D	501	7Z2	C20-C21	-2.79	1.38	1.43
2	В	501	7Z2	C40-C13	2.69	1.43	1.39
2	А	501	7Z2	C18-C17	2.65	1.58	1.50
2	С	501	7Z2	C39-C40	2.54	1.43	1.38
2	С	501	7Z2	C22-N26	-2.54	1.33	1.37
2	С	501	7Z2	C40-C13	2.54	1.43	1.39
2	D	501	7Z2	C34-N32	2.54	1.50	1.46
2	С	501	7Z2	C34-N32	2.49	1.50	1.46
2	A	501	7Z2	C3-C4	2.37	1.53	1.50
2	В	501	7Z2	C20-C21	-2.24	1.39	1.43
2	С	501	7Z2	C3-C4	2.20	1.53	1.50
2	С	501	7Z2	C18-C19	-2.09	1.51	1.53
2	С	501	7Z2	C21-C22	-2.08	1.39	1.42

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	С	501	7Z2	C15-C16-C17	-7.60	111.59	120.84
2	В	501	7Z2	C15-C16-C17	-7.57	111.63	120.84
2	В	501	7Z2	C5-C6-N2	-7.50	98.92	102.46
2	В	501	7Z2	O11-C1-N2	-7.40	111.38	121.78
2	С	501	7Z2	C39-C16-C17	7.22	129.61	120.84
2	D	501	7Z2	O11-C1-N2	-7.00	111.95	121.78
2	С	501	7Z2	C9-C10-C4	-5.51	114.67	119.47
2	С	501	7Z2	O11-C1-N2	-5.48	114.08	121.78
2	В	501	7Z2	C39-C16-C17	5.06	127.00	120.84
2	А	501	7Z2	C39-C16-C17	4.68	126.53	120.84
2	В	501	7Z2	C34-N32-N33	4.67	121.63	114.20
2	С	501	7Z2	C16-C17-N33	4.63	120.28	116.24
2	В	501	7Z2	C5-C7-N8	-4.58	118.04	124.46
2	В	501	7Z2	C40-C39-C16	-4.44	115.61	120.78
2	A	501	7Z2	C18-C19-C20	4.36	117.29	111.63
2	С	501	7Z2	C5-C7-N8	-4.28	118.47	124.46



Mol	Chain	Res	Type	Atoms	$\mathbf{Z} = \mathbf{Observed}(^{o})$		$Ideal(^{o})$
2	В	501	7Z2	C9-N8-C7	4.25	124.20	116.85
2	С	501	7Z2	C34-N32-N33	4.05	120.65	114.20
2	А	501	7Z2	C5-C6-N2	-3.99	100.58	102.46
2	D	501	7Z2	N12-C1-N2	3.64	120.05	115.89
2	В	501	7Z2	C9-C10-C4	-3.45	116.47	119.47
2	D	501	7Z2	C15-C16-C17	-3.42	116.67	120.84
2	D	501	7Z2	C9-N8-C7	3.41	122.74	116.85
2	В	501	7Z2	C39-C40-C13	3.37	124.19	120.30
2	В	501	7Z2	C18-C19-C20	3.28	115.88	111.63
2	С	501	7Z2	C39-C40-C13	3.20	124.00	120.30
2	В	501	7Z2	O11-C1-N12	3.15	130.60	123.61
2	С	501	7Z2	C40-C39-C16	-3.10	117.17	120.78
2	В	501	7Z2	C4-C3-N2	-3.09	101.00	102.46
2	D	501	7Z2	C16-C17-N33	3.05	118.90	116.24
2	D	501	7Z2	C39-C16-C17	2.97	124.45	120.84
2	С	501	7Z2	C27-N26-C22	2.97	121.53	116.93
2	А	501	7Z2	C15-C16-C17	-2.94	117.26	120.84
2	А	501	7Z2	C35-C34-N32	-2.94	106.35	112.26
2	А	501	7Z2	O11-C1-N2	-2.89	117.73	121.78
2	С	501	7Z2	C6-C5-C4	-2.88	108.25	110.53
2	С	501	7Z2	C14-C15-C16	2.85	124.10	120.78
2	А	501	7Z2	C16-C17-N33	2.83	118.71	116.24
2	В	501	7Z2	C29-C21-C20	-2.75	120.20	123.40
2	А	501	7Z2	C10-C9-N8	-2.74	118.86	123.62
2	С	501	7Z2	C21-C22-N26	-2.64	120.02	122.83
2	А	501	7Z2	C3-C4-C5	-2.63	108.45	110.53
2	D	501	7Z2	C27-N26-C22	2.54	120.87	116.93
2	А	501	7Z2	C34-N32-N33	2.52	118.22	114.20
2	D	501	7Z2	C20-C21-C22	2.39	120.63	117.47
2	D	501	7Z2	C10-C9-N8	-2.39	119.46	123.62
2	А	501	7Z2	C27-N26-C22	2.37	120.61	116.93
2	A	501	7Z2	C9-N8-C7	2.36	120.92	116.85
2	А	501	7Z2	C6-C5-C7	2.32	134.24	127.61
2	D	501	7Z2	C28-C27-N26	-2.30	120.42	123.94
2	D	501	7Z2	C5-C7-N8	-2.26	121.30	124.46
2	D	501	7Z2	C28-C29-C21	-2.22	117.82	120.89
2	В	501	7Z2	C20-C21-C22	2.20	120.37	117.47
2	С	501	7Z2	C13-N12-C1	2.09	130.32	126.12
2	A	501	7Z2	C9-C10-C4	2.08	121.28	119.47
2	D	501	7Z2	C29-C21-C20	-2.06	121.00	123.40
2	В	501	7Z2	C27-N26-C22	2.05	120.10	116.93
2	В	501	7Z2	C35-C34-N32	2.05	116.37	112.26



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	501	7Z2	C9-N8-C7	2.01	120.32	116.85

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	501	7Z2	C35-C34-N32-N33
2	В	501	7Z2	C35-C34-N32-C30
2	D	501	7Z2	C30-C19-C20-C21
5	С	504	GOL	C1-C2-C3-O3
5	С	507	GOL	C1-C2-C3-O3
2	А	501	7Z2	N32-C34-C35-C36
2	В	501	7Z2	C34-C35-C36-C37
2	В	501	7Z2	N32-C34-C35-C36
2	D	501	7Z2	N32-C34-C35-C36
5	С	504	GOL	O1-C1-C2-C3
2	D	501	7Z2	C34-C35-C36-C37
5	С	504	GOL	O2-C2-C3-O3
2	С	501	7Z2	N32-C34-C35-C36
5	С	507	GOL	O2-C2-C3-O3
2	А	501	7Z2	C30-C19-C20-C25
2	В	501	7Z2	C30-C19-C20-C25
2	С	501	7Z2	C30-C19-C20-C25
2	D	501	7Z2	C30-C19-C20-C25
2	А	501	7Z2	C30-C19-C20-C21
2	В	501	7Z2	C30-C19-C20-C21
2	С	501	7Z2	C30-C19-C20-C21
2	В	501	7Z2	C35-C36-C37-N38
2	В	501	7Z2	C15-C16-C17-N33
5	С	504	GOL	O1-C1-C2-O2
2	D	501	7Z2	C35-C34-N32-N33
2	С	501	7Z2	C34-C35-C36-C37
2	А	501	7Z2	C35-C34-N32-C30
2	С	501	7Z2	C15-C16-C17-N33

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	501	7Z2	4	0
5	С	507	GOL	2	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	PO4	5	0
2	D	501	7Z2	4	0
3	В	502	PO4	2	0
3	С	502	PO4	1	0
2	С	501	7Z2	5	0
2	В	501	7Z2	5	0

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The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

















5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RS	\mathbf{RZ} >	2	$OWAB(Å^2)$	Q<0.9
1	А	463/492~(94%)	0.72	22 (4%)	30	41	8, 19, 34, 56	0
1	В	463/492~(94%)	0.75	24 (5%)	27	38	8, 19, 35, 50	0
1	С	464/492~(94%)	0.66	16 (3%)	45	55	8, 17, 33, 56	0
1	D	463/492~(94%)	0.69	21 (4%)	33	44	6, 16, 33, 47	0
All	All	1853/1968~(94%)	0.70	83 (4%)	33	44	6, 18, 34, 56	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	75	VAL	6.0
1	В	409	LEU	5.7
1	С	454	GLY	4.1
1	А	181	GLY	4.1
1	А	451	GLU	3.4
1	С	242	VAL	3.3
1	А	295	LEU	3.3
1	А	343	LEU	3.2
1	D	105	LEU	3.2
1	В	108	TYR	3.2
1	В	161	VAL	3.1
1	D	83	ALA	3.1
1	D	74	VAL	3.1
1	А	462	PHE	3.1
1	В	230	TYR	3.0
1	В	406	THR	3.0
1	В	29	ASN	3.0
1	С	236	PRO	2.9
1	В	110	GLY	2.9
1	А	236	PRO	2.9
1	А	338	SER	2.9



Mol	Chain	Res	Type	RSRZ	
1	В	304	THR	2.9	
1	А	261	ALA	2.8	
1	D	23	TYR	2.7	
1	D	453	TYR	2.6	
1	В	76	THR	2.6	
1	D	181	GLY	2.6	
1	В	77	LYS	2.6	
1	D	409	LEU	2.6	
1	В	467	VAL	2.5	
1	А	387	LEU	2.5	
1	А	397	CYS	2.5	
1	В	103	TYR	2.5	
1	С	205	GLY	2.5	
1	А	95	VAL	2.5	
1	С	108	TYR	2.5	
1	С	467	VAL	2.5	
1	В	204	ALA	2.4	
1	D	173	ALA	2.4	
1	D	113 PRO		2.4	
1	В	198	VAL	2.4	
1	В	334[A]	VAL	2.4	
1	А	226	LEU	2.3	
1	В	450	LEU	2.3	
1	С	75	VAL	2.3	
1	А	453	TYR	2.3	
1	В	92	GLN	2.3	
1	А	480	ALA	2.3	
1	А	175	TYR	2.3	
1	С	190	LEU	2.3	
1	D	334[A]	VAL	2.3	
1	А	108	TYR	2.3	
1	С	271	SER	2.3	
1	А	348	LEU	2.2	
1	А	161	VAL	2.2	
1	С	435	THR	2.2	
1	D	99	LYS	2.2	
1	А	323	LYS	2.2	
1	D	108	TYR	2.2	
1	В	160	THR	2.2	
1	D	156	TRP	2.2	
1	D	208	ALA	2.1	
1	В	351	ILE	2.1	



Mol	Chain	Res	Type	RSRZ	
1	В	387	LEU	2.1	
1	А	150	THR	2.1	
1	D	337	ASN	2.1	
1	В	261	ALA	2.1	
1	С	419	ALA	2.1	
1	D	103	TYR	2.1	
1	D	96	PHE	2.1	
1	D	159	ILE	2.1	
1	С	322	LEU	2.1	
1	С	482	LEU	2.1	
1	В	159	ILE	2.1	
1	D	81	GLN	2.1	
1	С	343	LEU	2.0	
1	В	382	SER	2.0	
1	D	436	PRO	2.0	
1	С	37	PHE	2.0	
1	В	28	28 PRO		
1	С	193	PHE	2.0	
1	А	23	TYR	2.0	
1	А	82	GLU	2.0	

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
5	GOL	С	507	6/6	0.71	0.34	$24,\!36,\!41,\!43$	0
2	7Z2	D	501	40/40	0.81	0.23	12,22,38,45	0
2	7Z2	А	501	40/40	0.83	0.23	8,26,40,50	0



7PPI

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
2	7Z2	В	501	40/40	0.84	0.21	6,13,34,41	0
5	GOL	С	504	6/6	0.87	0.18	18,24,29,31	0
2	7Z2	С	501	40/40	0.87	0.19	8,13,19,21	0
3	PO4	D	502	5/5	0.90	0.19	21,25,36,41	0
3	PO4	С	502	5/5	0.93	0.17	17,18,21,27	0
5	GOL	А	504	6/6	0.93	0.13	21,23,24,24	0
4	CL	С	503	1/1	0.95	0.22	31,31,31,31	0
3	PO4	А	502	5/5	0.96	0.12	20,22,24,25	0
4	CL	А	503	1/1	0.96	0.26	23,23,23,23	0
4	CL	А	506	1/1	0.97	0.10	31,31,31,31	0
4	CL	С	506	1/1	0.98	0.22	22,22,22,22	0
4	CL	В	503	1/1	0.98	0.19	29,29,29,29	0
3	PO4	В	502	5/5	0.98	0.16	13,17,24,26	0
4	CL	С	505	1/1	0.98	0.12	18,18,18,18	0
4	CL	A	505	1/1	0.99	0.09	22,22,22,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











6.5 Other polymers (i)

There are no such residues in this entry.

